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LOGINID:SSPTAEAL1624

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS 1   Web Page for STN Seminar Schedule – N. America
 NEWS 2 AUG 06   CAS REGISTRY enhanced with new experimental property tags
 NEWS 3 AUG 06   FSTA enhanced with new thesaurus edition
 NEWS 4 AUG 13   CA/CAplus enhanced with additional kind codes for granted
                   patents
 NEWS 5 AUG 20   CA/CAplus enhanced with CAS indexing in pre-1907 records
 NEWS 6 AUG 27   Full-text patent databases enhanced with predefined
                   patent family display formats from INPADOCDB
 NEWS 7 AUG 27   USPATOLD now available on STN
 NEWS 8 AUG 28   CAS REGISTRY enhanced with additional experimental
                   spectral property data
 NEWS 9 SEP 07   STN AnaVist, Version 2.0, now available with Derwent
                   World Patents Index
 NEWS 10 SEP 13   FORIS renamed to SOFIS
 NEWS 11 SEP 13   INPADOCDB enhanced with monthly SDI frequency
 NEWS 12 SEP 17   CA/CAplus enhanced with printed CA page images from
                   1967–1998
 NEWS 13 SEP 17   CAplus coverage extended to include traditional medicine
                   patents
 NEWS 14 SEP 24   EMBASE, EMBAL, and LEMBASE reloaded with enhancements
 NEWS 15 OCT 02   CA/CAplus enhanced with pre-1907 records from Chemisches
                   Zentralblatt
 NEWS 16 OCT 19   BEILSTEIN updated with new compounds
 NEWS 17 NOV 15   Derwent Indian patent publication number format enhanced
 NEWS 18 NOV 19   WPIX enhanced with XML display format
 NEWS 19 NOV 30   ICSD reloaded with enhancements
 NEWS 20 DEC 04   LINPADOCDB now available on STN
 NEWS 21 DEC 14   BEILSTEIN pricing structure to change
 NEWS 22 DEC 17   USPATOLD added to additional database clusters
 NEWS 23 DEC 17   IMSDRUGCONF removed from database clusters and STN
 NEWS 24 DEC 17   DGENE now includes more than 10 million sequences
 NEWS 25 DEC 17   TOXCENTER enhanced with 2008 MeSH vocabulary in
                   MEDLINE segment
 NEWS 26 DEC 17   MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
 NEWS 27 DEC 17   CA/CAplus enhanced with new custom IPC display formats
 NEWS 28 DEC 17   STN Viewer enhanced with full-text patent content
                   from USPATOLD

 NEWS EXPRESS 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2,
               CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

 NEWS HOURS   STN Operating Hours Plus Help Desk Availability

* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 18:00:07 ON 17 DEC 2007

=> file reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                  ENTRY   SESSION
FULL ESTIMATED COST   0.21   0.21

FILE 'REGISTRY' ENTERED AT 18:00:12 ON 17 DEC 2007
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 16 DEC 2007 HIGHEST RN 958294-65-0
DICTIONARY FILE UPDATES: 16 DEC 2007 HIGHEST RN 958294-65-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10588012election.str
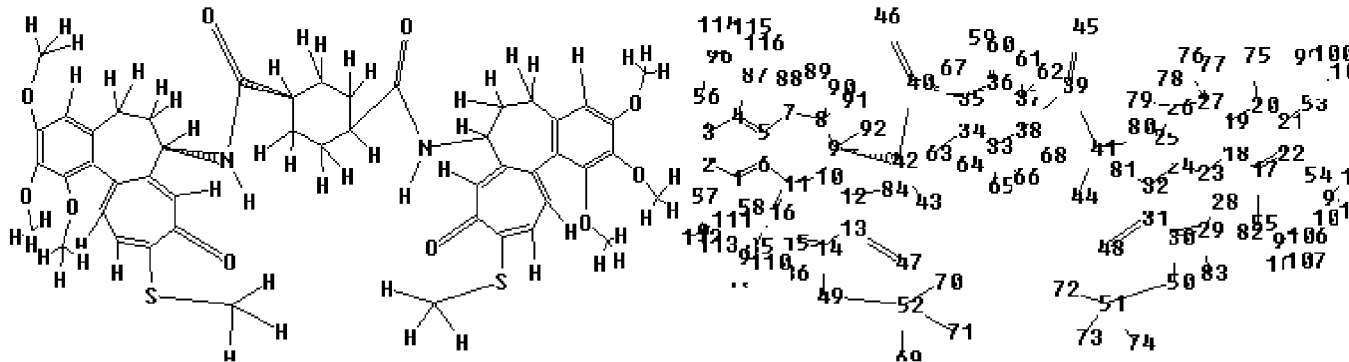
```
chain nodes :
39   40   41   42   43   44   45   46   47   48   49   50   51   52   53   54   55   56   57   58   59
60   61   62   63   64   65   66   67   68   69   70   71   72   73   74   75   76   77   78   79   80
81   82   83
84   85   86   87   88   89   90   91   92   93   94   95   96   97   98   99   100  101  102  103
104  105  106
107  108  109  110  111  112  113  114  115  116
ring nodes :
1   2   3   4   5   6   7   8   9   10   11   12   13   14   15   16   17   18   19   20   21   22   23
24   25   26   27   28   29   30   31   32   33   34   35   36   37   38
chain bonds :
1-58   2-57   3-56   4-87   7-88   7-89   8-90   8-91   9-42   9-92   12-84   13-47   14-49
15-86   16-85   17-55   20-75   21-53   22-54   25-41   25-80   26-78   26-79   27-76   27-77
28-82   29-83   30-50
31-48   32-81   33-65   33-66   34-63   34-64   35-40   35-67   36-59   36-60   37-61   37-62
38-39   38-68
39-45   39-41   40-42   40-46   41-44   42-43   49-52   50-51   51-72   51-73   51-74   52-69
52-70   52-71
53-93   54-94   55-95   56-96   57-98   58-97   93-99   93-100   93-101   94-102   94-103
94-104   95-105
95-106   95-107   96-114   96-115   96-116   97-108   97-109   97-110   98-111   98-112   98-
113
ring bonds :
1-2   1-6   2-3   3-4   4-5   5-6   5-7   6-11   7-8   8-9   9-10   10-11   10-12   11-16   12-13
13-14   14-15   15-16   17-18   17-22   18-19   18-23   19-20   19-27   20-21   21-22   23-24
23-28   24-25
24-32   25-26   26-27   28-29   29-30   30-31   31-32   33-34   33-38   34-35   35-36   36-37
37-38
exact/norm bonds :
1-58   2-57   3-56   9-42   13-47   14-49   17-55   21-53   22-54   25-41   30-50   31-48   39-
45
39-41   40-42   40-46   49-52   50-51   53-93   54-94   55-95   56-96   57-98   58-97
exact bonds :
4-87   5-7   6-11   7-8   7-88   7-89   8-9   8-90   8-91   9-10   9-92   10-11   10-12   11-16
12-13   12-84   13-14   14-15   15-16   15-86   16-85   18-23   19-27   20-75   23-24   23-28
24-25   24-32
25-26   25-80   26-27   26-78   26-79   27-76   27-77   28-29   28-82   29-30   29-83   30-31
31-32   32-81
33-34   33-38   33-65   33-66   34-35   34-63   34-64   35-36   35-40   35-67   36-37   36-59
36-60   37-38
37-61   37-62   38-39   38-68   41-44   42-43   51-72   51-73   51-74   52-69   52-70   52-71
93-99   93-100
93-101   94-102   94-103   94-104   95-105   95-106   95-107   96-114   96-115   96-116   97-
108   97-109   97-110
98-111   98-112   98-113
normalized bonds :
1-2   1-6   2-3   3-4   4-5   5-6   17-18   17-22   18-19   19-20   20-21   21-22
isolated ring systems :
containing 1 : 17 : 33 :


Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom   10:Atom
11:Atom   12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:Atom   18:Atom   19:Atom
20:Atom   21:Atom
22:Atom   23:Atom   24:Atom   25:Atom   26:Atom   27:Atom   28:Atom   29:Atom   30:Atom
31:Atom   32:Atom
33:Atom   34:Atom   35:Atom   36:Atom   37:Atom   38:Atom   39:CLASS   40:CLASS   41:CLASS
```

```
42:CLASS    43:CLASS
44:CLASS    45:CLASS    46:CLASS    47:CLASS    48:CLASS    49:CLASS    50:CLASS    51:CLASS
52:CLASS    53:CLASS
54:CLASS    55:CLASS    56:CLASS    57:CLASS    58:CLASS    59:CLASS    60:CLASS    61:CLASS
62:CLASS    63:CLASS
64:CLASS    65:CLASS    66:CLASS    67:CLASS    68:CLASS    69:CLASS    70:CLASS    71:CLASS
72:CLASS    73:CLASS
74:CLASS    75:CLASS    76:CLASS    77:CLASS    78:CLASS    79:CLASS    80:CLASS    81:CLASS
82:CLASS    83:CLASS
84:CLASS    85:CLASS    86:CLASS    87:CLASS    88:CLASS    89:CLASS    90:CLASS    91:CLASS
92:CLASS
93:CLASS    94:CLASS    95:CLASS    96:CLASS    97:CLASS    98:CLASS    99:CLASS    100:CLASS
101:CLASS   102:CLASS
103:CLASS   104:CLASS   105:CLASS   106:CLASS   107:CLASS   108:CLASS   109:CLASS
110:CLASS   111:CLASS
112:CLASS   113:CLASS   114:CLASS   115:CLASS   116:CLASS

Stereo Bonds:

40-35 (Single Hash).
42-9 (Single Hash).


Stereo Chiral Centers:

9     (Parity=Even)
35     (Parity=Even)

Stereo RSS Sets:

Type=Relative (Default). 2 Nodes= 9 35
L1        STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1                STR
```
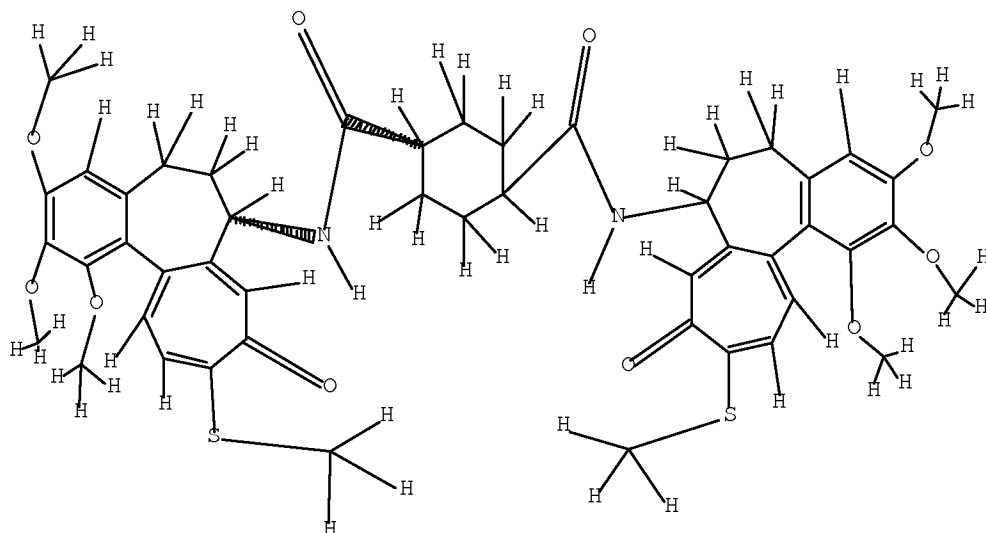

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1 full
FULL SEARCH INITIATED 18:01:03 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -        51 TO ITERATE

100.0% PROCESSED        51 ITERATIONS                           1 ANSWERS
SEARCH TIME: 00.00.01


L2              1 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                   ENTRY      SESSION
FULL ESTIMATED COST                              172.55       172.76


FILE 'CAPLUS' ENTERED AT 18:01:09 ON 17 DEC 2007
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```

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FILE COVERS 1907 - 17 Dec 2007  VOL 147 ISS 26
FILE LAST UPDATED: 16 Dec 2007  (20071216/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l2 full
L3              1 L2

=> d ibib abs hitstr

L3   ANSWER 1 OF 1   CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:          2005:823659  CAPLUS  Full-text
DOCUMENT NUMBER:           143:212050
TITLE:                     Preparation of N-deacetylthiocolchicine derivatives
                           for use in antiproliferative, anti-inflammatory,
                           antiarthritic and antiviral pharmaceutical
                           compositions
INVENTOR(S):               Bombardelli, Ezio; Fontana, Gabriele
PATENT ASSIGNEE(S):        Indena S.p.A., Italy
SOURCE:                    PCT Int. Appl., 15 pp.
                           CODEN: PIXXD2
DOCUMENT TYPE:             Patent
LANGUAGE:                  English
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:
```
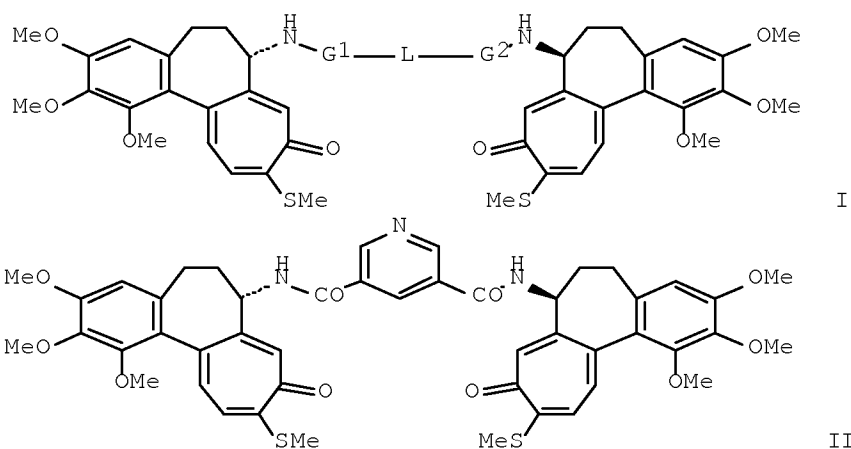
```
PATENT NO.              KIND   DATE        APPLICATION NO.          DATE
---------------         ----   --------    --------------------     --------
WO 2005075418           A2     20050818    WO 2005-EP987            20050201
WO 2005075418           A3     20070503
     W:   AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
          CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
          GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
          LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
          NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
          TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, SM
     RW:  BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
          AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
          EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
          RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
          MR, NE, SN, TD, TG, AP, EA, EP, OA
AU 2005211501           A1     20050818    AU 2005-211501           20050201
CA 2555058              A1     20050818    CA 2005-2555058          20050201
EP 1711461              A2     20061018    EP 2005-707124           20050201
     R:   AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
          IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK,
          BA, HR, IS, YU
CN 1972908              A      20070530    CN 2005-80003821         20050201
JP 2007520486           T      20070726    JP 2006-550141           20050201
NO 2006003509           A      20060801    NO 2006-3509             20060801
IN 2006DN04429          A      20070622    IN 2006-DN4429           20060801
US 2007191486           A1     20070816    US 2006-588012           20061006
PRIORITY APPLN. INFO.:                     IT 2004-MI164        A   20040203
                                           WO 2005-EP987        W   20050201

OTHER SOURCE(S):        CASREACT 143:212050; MARPAT 143:212050
GI
```


I

II

AB   N-Deacetylthiocolchicine derivs., such as I [G1 = -CO-, -CONH-, -CR2-; G2 = -
      CO-, -NHCO-, -CR2-; L = linking group, such as alkylene, phenylene,
      cyclohexanediyl, pyridinediyl, piperidinediyl, piperazinediyl; R = H, alkyl],
      were prepared for therapeutic use as antitumor, antiproliferative, anti-

inflammatory, antiarthritic and antiviral agents. Thus, N-deacetylthiocolchicine derivative II was prepared via an amidation reaction of N-deacetylthiocolchicine with 3,5-pyridinedicarboxylic acid using DMAP and DCC in CH2Cl2. The prepared N-deacetylthiocolchicine derivs. were assayed for cytotoxic activity against human cancer cell lines, such as MCF7 breast cancer cells and A2780 ovarial cancer cells.

IT   862502-66-7P

    RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

       (preparation of N-deacetylthiocolchicine derivs. for use in antiproliferative, anti-inflammatory, antiarthritic and antiviral pharmaceutical compns.)

RN   862502-66-7 CAPLUS

CN   1,4-Cyclohexanedicarboxamide, N,N'-bis[(7S)-5,6,7,9-tetrahydro-1,2,3-trimethoxy-10-(methylthio)-9-oxobenzo[a]heptalen-7-yl]-, trans- (9CI) (CA INDEX NAME)
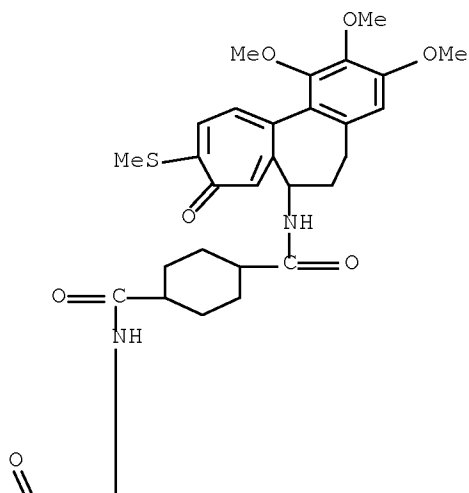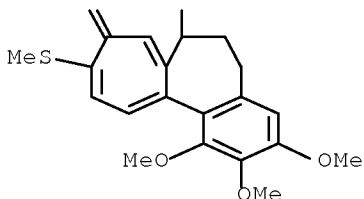
=> file reg

```
COST IN U.S. DOLLARS                        SINCE FILE      TOTAL
                                            ENTRY          SESSION
FULL ESTIMATED COST                         15.14          187.90


DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)  SINCE FILE      TOTAL
                                            ENTRY          SESSION
CA SUBSCRIBER PRICE                         -0.78          -0.78
```

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STRUCTURE FILE UPDATES: 16 DEC 2007 HIGHEST RN 958294-65-0
DICTIONARY FILE UPDATES: 16 DEC 2007 HIGHEST RN 958294-65-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

   Please note that search-term pricing does apply when
   conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10588012nonitrogen.str


```
chain nodes :
33   34   35   36   37   38   39   40   41   42   43   44   45   46   47   48   49   50   51   52   53
54   55   56   57   58   59   60   61   62   63   64   65   66   67   68   69   70   71   72   73   74
75   76   77
78   79   80   81   82   83   84   85   86   87   88   89   90   91   92   93   94   95   96   97   98
99   100  102
ring nodes :
1    2    3    4    5    6    7    8    9    10   11   12   13   14   15   16   17   18   19   20   21   22   23
24   25   26   27   28   29   30   31   32
chain bonds :
1-52   2-51   3-50   4-71   7-72   7-73   8-74   8-75   9-36   9-76   12-68   13-41   14-43
```

```
15-70   16-69   17-49   20-59   21-47   22-48   25-35   25-64   26-62   26-63   27-60   27-61
28-66   29-67   30-44
31-42   32-65   33-39   33-35   33-102   34-40   34-36   34-102   35-38   36-37   43-46   44-
45   45-56
45-57   45-58   46-53   46-54   46-55   47-77   48-78   49-79   50-80   51-82   52-81   77-83
77-84   77-85   78-86
78-87   78-88   79-89   79-90   79-91   80-98   80-99   80-100   81-92   81-93   81-94   82-95
82-96   82-97
```

ring bonds :
```
1-2   1-6   2-3   3-4   4-5   5-6   5-7   6-11   7-8   8-9   9-10   10-11   10-12   11-16   12-13
13-14   14-15   15-16   17-18   17-22   18-19   18-23   19-20   19-27   20-21   21-22   23-24
23-28   24-25
24-32   25-26   26-27   28-29   29-30   30-31   31-32
```
exact/norm bonds :
```
1-52   2-51   3-50   9-36   13-41   14-43   17-49   21-47   22-48   25-35   30-44   31-42   33-
39
33-35   33-102   34-40   34-36   34-102   43-46   44-45   47-77   48-78   49-79   50-80   51-
82   52-81
```

exact bonds :
```
4-71   5-7   6-11   7-8   7-72   7-73   8-9   8-74   8-75   9-10   9-76   10-11   10-12   11-16
12-13   12-68   13-14   14-15   15-16   15-70   16-69   18-23   19-27   20-59   23-24   23-28
24-25   24-32
25-26   25-64   26-27   26-62   26-63   27-60   27-61   28-29   28-66   29-30   29-67   30-31
31-32   32-65
35-38   36-37   45-56   45-57   45-58   46-53   46-54   46-55   77-83   77-84   77-85   78-86
78-87   78-88
79-89   79-90   79-91   80-98   80-99   80-100   81-92   81-93   81-94   82-95   82-96   82-97
```
normalized bonds :
```
1-2   1-6   2-3   3-4   4-5   5-6   17-18   17-22   18-19   19-20   20-21   21-22
```
isolated ring systems :
containing 1 : 17 :

Match level :
```
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom   10:Atom
11:Atom   12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:Atom   18:Atom   19:Atom
20:Atom   21:Atom
22:Atom   23:Atom   24:Atom   25:Atom   26:Atom   27:Atom   28:Atom   29:Atom   30:Atom
31:Atom   32:Atom
33:CLASS   34:CLASS   35:CLASS   36:CLASS   37:CLASS   38:CLASS   39:CLASS   40:CLASS
41:CLASS   42:CLASS
43:CLASS   44:CLASS   45:CLASS   46:CLASS   47:CLASS   48:CLASS   49:CLASS   50:CLASS
51:CLASS   52:CLASS
53:CLASS   54:CLASS   55:CLASS   56:CLASS   57:CLASS   58:CLASS   59:CLASS   60:CLASS
61:CLASS   62:CLASS
63:CLASS   64:CLASS   65:CLASS   66:CLASS   67:CLASS   68:CLASS   69:CLASS   70:CLASS
71:CLASS   72:CLASS
73:CLASS   74:CLASS   75:CLASS   76:CLASS   77:CLASS   78:CLASS   79:CLASS   80:CLASS
81:CLASS   82:CLASS
83:CLASS   84:CLASS   85:CLASS   86:CLASS   87:CLASS   88:CLASS   89:CLASS   90:CLASS
91:CLASS   92:CLASS
93:CLASS   94:CLASS   95:CLASS   96:CLASS   97:CLASS   98:CLASS   99:CLASS   100:CLASS
102:Atom
```

Stereo Bonds:

36-9 (Single Hash).

Stereo Chiral Centers:

9   (Parity=Don't Care)

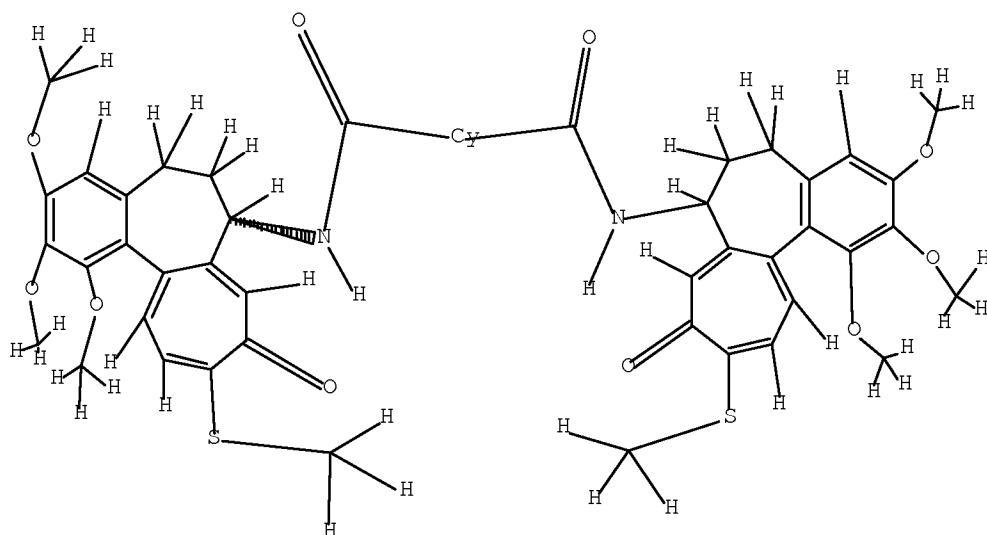Stereo RSS Sets:

Type=Relative (Default). 1 Nodes= 9
L4   STRUCTURE UPLOADED

=> d l4
L4 HAS NO ANSWERS
L4   STR

Structure attributes must be viewed using STN Express query preparation.

=> s l4 full
FULL SEARCH INITIATED 18:14:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED –   51 TO ITERATE

100.0% PROCESSED   51 ITERATIONS   4 ANSWERS
SEARCH TIME: 00.00.01

L5   4 SEA SSS FUL L4

=> file caplus
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                    ENTRY   SESSION
FULL ESTIMATED COST   172.10   360.00

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)   SINCE FILE   TOTAL
                                                    ENTRY   SESSION
CA SUBSCRIBER PRICE   0.00   -0.78

FILE 'CAPLUS' ENTERED AT 18:14:23 ON 17 DEC 2007
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FILE COVERS 1907 - 17 Dec 2007 VOL 147 ISS 26
FILE LAST UPDATED: 16 Dec 2007 (20071216/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

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=> s l5 full
L6   2 L5

=> d ibib abs hitstr tot

L6   ANSWER 1 OF 2   CAPLUS   COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:847858   CAPLUS Full-text
DOCUMENT NUMBER: 145:278405
TITLE: Drugs with improved hydrophobicity for incorporation
                         in medical devices
INVENTOR(S):   Desai, Neil P.; Tao, Chunlin; Yu, Chengzhi; Wang,
                         Qinwei; Soon-Shiong, Patrick
PATENT ASSIGNEE(S):   American Bioscience, Inc., USA
SOURCE: PCT Int. Appl., 43pp.
                         CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

       PATENT NO.   KIND   DATE   APPLICATION NO.   DATE
       ---------------   ----   --------   --------------------   --------
       WO 2006089207   A2   20060824   WO 2006-US5799   20060221
       WO 2006089207   A3   20070518
          W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
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            BA, HR, MK, YU
PRIORITY APPLN. INFO.:   US 2005-654175P   P 20050218
                                            WO 2006-US5799   W 20060221
OTHER SOURCE(S):   MARPAT 145:278405
AB   The invention provides a medical device comprising a hydrophobic analog of a
      medicament known to inhibit cell proliferation and migration. The invention
      also provides a method of treating a narrowing in a body passageway comprising
      placing an implantable medical device comprising a hydrophobic analog of a
      medicament known to inhibit cell proliferation and migration. The medicaments
      can be incorporated within or coated on the device. The invention further
      provides hydrophobic analogs of medicaments known to inhibit cell
      proliferation and migration.
IT   862502-65-6P 906649-27-2P
      RL: PRP (Properties); PUR (Purification or recovery); SPN (Synthetic
      preparation); THU (Therapeutic use); BIOL (Biological study); PREP
      (Preparation); USES (Uses)
          (drugs with improved hydrophobicity for incorporation in medical
          devices)
RN   862502-65-6 CAPLUS
CN   3,5-Pyridinedicarboxamide, N,N'-bis[(7S)-5,6,7,9-tetrahydro-1,2,3-
      trimethoxy-10-(methylthio)-9-oxobenzo[a]heptalen-7-yl]- (9CI) (CA INDEX
      NAME)

Absolute stereochemistry.
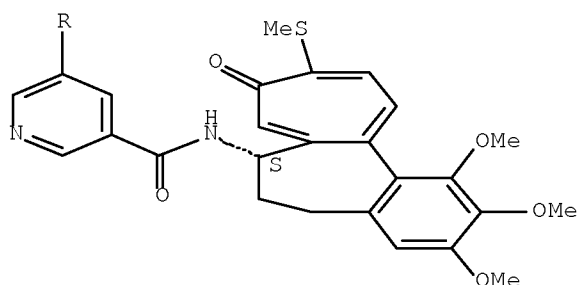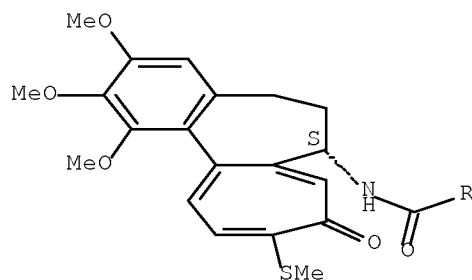
PAGE 1-A

PAGE 2-A

RN   906649-27-2 CAPLUS
CN   1,3-Cyclohexanedicarboxamide, N,N'-bis[(7S)-5,6,7,9-tetrahydro-1,2,3-
      trimethoxy-10-(methylthio)-9-oxobenzo[a]heptalen-7-yl]- (9CI) (CA INDEX
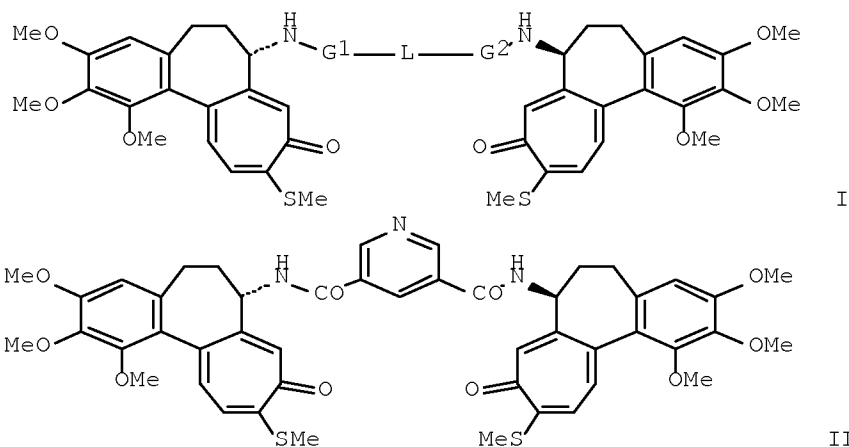   NAME)
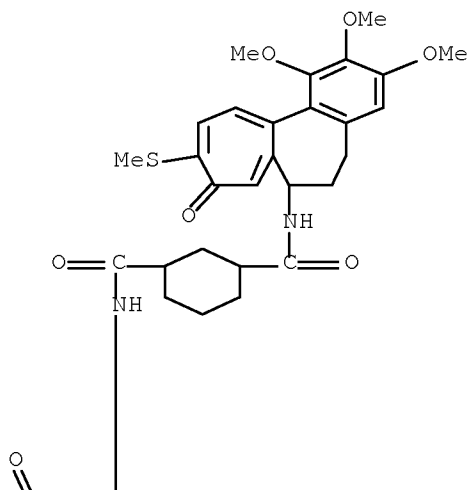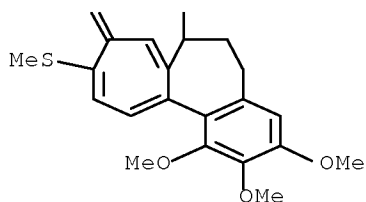
L6   ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:823659 CAPLUS Full-text
DOCUMENT NUMBER: 143:212050
TITLE: Preparation of N-deacetylthiocolchicine derivatives
                          for use in antiproliferative, anti-inflammatory,
                          antiarthritic and antiviral pharmaceutical
                          compositions
INVENTOR(S):   Bombardelli, Ezio; Fontana, Gabriele
PATENT ASSIGNEE(S):   Indena S.p.A., Italy
SOURCE: PCT Int. Appl., 15 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

AB   N-Deacetylthiocolchicine derivs., such as I [G1 = -CO-, -CONH-, -CR2-; G2 = -
      CO-, -NHCO-, -CR2-; L = linking group, such as alkylene, phenylene,
      cyclohexanediyl, pyridinediyl, piperidinediyl, piperazinediyl; R = H, alkyl],
      were prepared for therapeutic use as antitumor, antiproliferative, anti-
      inflammatory, antiarthritic and antiviral agents. Thus, N-
      deacetylthiocolchicine derivative II was prepared via an amidation reaction of

N-deacetylthiocolchicine with 3,5-pyridinedicarboxylic acid using DMAP and DCC
in CH2Cl2. The prepared N-deacetylthiocolchicine derivs. were assayed for
cytotoxic activity against human cancer cell lines, such as MCF7 breast cancer
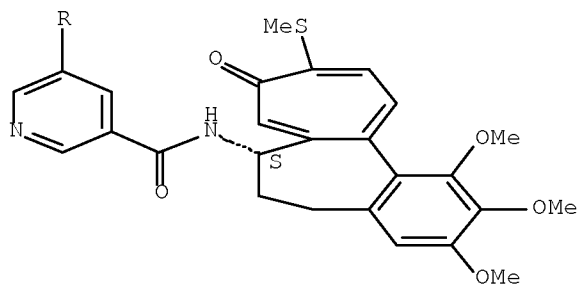cells and A2780 ovarial cancer cells.

IT   862502-65-6P
      RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
      preparation); THU (Therapeutic use); BIOL (Biological study); PREP
      (Preparation); RACT (Reactant or reagent); USES (Uses)
          (preparation of N-deacetylthiocolchicine derivs. for use in
          antiproliferative, anti-inflammatory, antiarthritic and antiviral
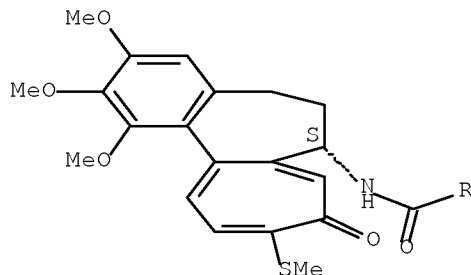   pharmaceutical compns.)
RN   862502-65-6 CAPLUS
CN   3,5-Pyridinedicarboxamide, N,N'-bis[(7S)-5,6,7,9-tetrahydro-1,2,3-
      trimethoxy-10-(methylthio)-9-oxobenzo[a]heptalen-7-yl]- (9CI) (CA INDEX
      NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 2-A

IT   862502-65-6DP, complex with human albumin 862502-66-7P
      862502-67-8P
      RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
      (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
      (Uses)
          (preparation of N-deacetylthiocolchicine derivs. for use in
          antiproliferative, anti-inflammatory, antiarthritic and antiviral
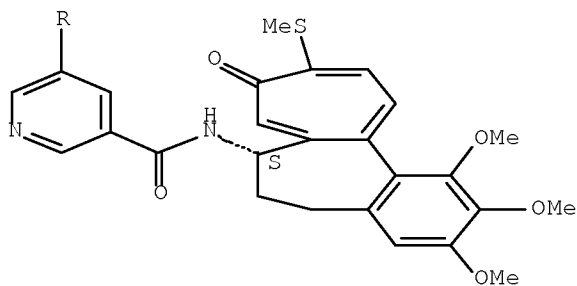   pharmaceutical compns.)
RN   862502-65-6 CAPLUS
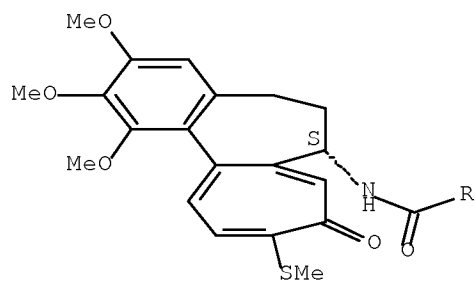CN   3,5-Pyridinedicarboxamide, N,N'-bis[(7S)-5,6,7,9-tetrahydro-1,2,3-

trimethoxy-10-(methylthio)-9-oxobenzo[a]heptalen-7-yl]- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.

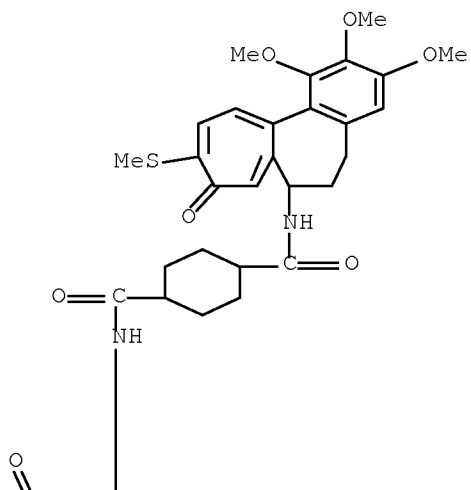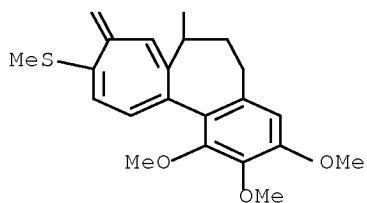RN   862502-66-7 CAPLUS
CN   1,4-Cyclohexanedicarboxamide, N,N'-bis[(7S)-5,6,7,9-tetrahydro-1,2,3-
      trimethoxy-10-(methylthio)-9-oxobenzo[a]heptalen-7-yl]-, trans- (9CI) (CA
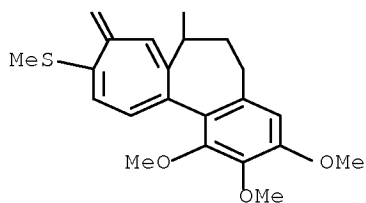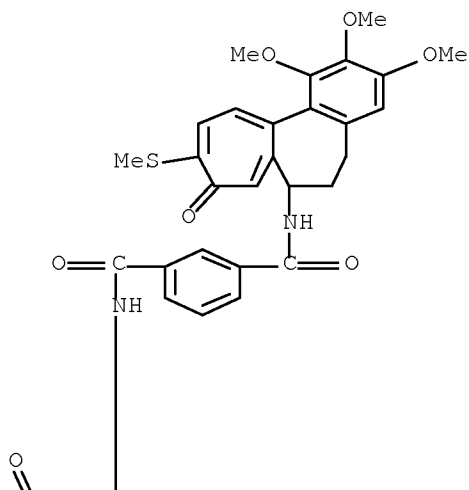   INDEX NAME)

RN   862502-67-8 CAPLUS
CN   1,3-Benzenedicarboxamide, N,N'-bis[(7S)-5,6,7,9-tetrahydro-1,2,3-
      trimethoxy-10-(methylthio)-9-oxobenzo[a]heptalen-7-yl]- (9CI) (CA INDEX
      NAME)

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                                                 ENTRY        SESSION
FULL ESTIMATED COST                              17.12        377.12


DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)     SINCE FILE      TOTAL
                                                 ENTRY        SESSION
CA SUBSCRIBER PRICE                              -1.56         -2.34
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DICTIONARY FILE UPDATES: 16 DEC 2007 HIGHEST RN 958294-65-0

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DICTIONARY FILE UPDATES: 16 DEC 2007 HIGHEST RN 958294-65-0

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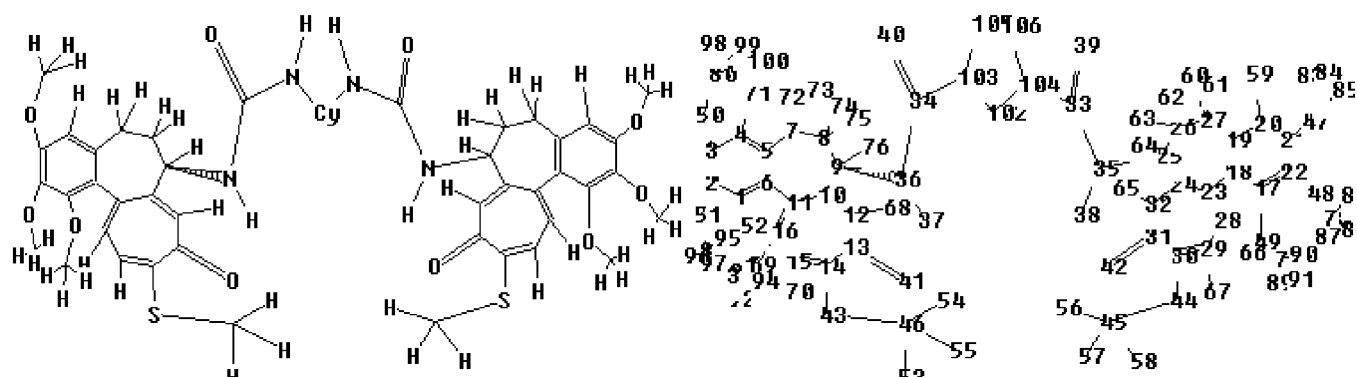
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predicted properties as well as tags indicating availability of
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http://www.cas.org/support/stngen/stndoc/properties.html

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chain nodes :
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54   55   56   57   58   59   60   61   62   63   64   65   66   67   68   69   70   71   72   73   74
75   76   77
78   79   80   81   82   83   84   85   86   87   88   89   90   91   92   93   94   95   96   97   98
99   100   102   103
104   105   106
ring nodes :
1   2   3   4   5   6   7   8   9   10   11   12   13   14   15   16   17   18   19   20   21   22   23
24   25   26   27   28   29   30   31   32
chain bonds :
1-52   2-51   3-50   4-71   7-72   7-73   8-74   8-75   9-36   9-76   12-68   13-41   14-43
15-70   16-69   17-49   20-59   21-47   22-48   25-35   25-64   26-62   26-63   27-60   27-61
28-66   29-67   30-44
31-42   32-65   33-39   33-35   33-104   34-40   34-36   34-103   35-38   36-37   43-46   44-
45   45-56
45-57   45-58   46-53   46-54   46-55   47-77   48-78   49-79   50-80   51-82   52-81   77-83
77-84   77-85   78-86
78-87   78-88   79-89   79-90   79-91   80-98   80-99   80-100   81-92   81-93   81-94   82-95
82-96   82-97
102-103   102-104   103-105   104-106
ring bonds :
1-2   1-6   2-3   3-4   4-5   5-6   5-7   6-11   7-8   8-9   9-10   10-11   10-12   11-16   12-13
13-14   14-15   15-16   17-18   17-22   18-19   18-23   19-20   19-27   20-21   21-22   23-24
23-28   24-25
24-32   25-26   26-27   28-29   29-30   30-31   31-32
exact/norm bonds :
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39
33-35   33-104   34-40   34-36   34-103   43-46   44-45   47-77   48-78   49-79   50-80   51-
82   52-81
102-103   102-104
exact bonds :
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12-13   12-68   13-14   14-15   15-16   15-70   16-69   18-23   19-27   20-59   23-24   23-28
24-25   24-32
25-26   25-64   26-27   26-62   26-63   27-60   27-61   28-29   28-66   29-30   29-67   30-31
31-32   32-65
35-38   36-37   45-56   45-57   45-58   46-53   46-54   46-55   77-83   77-84   77-85   78-86
78-87   78-88
79-89   79-90   79-91   80-98   80-99   80-100   81-92   81-93   81-94   82-95   82-96   82-97
103-105   104-106

normalized bonds :
1-2   1-6   2-3   3-4   4-5   5-6   17-18   17-22   18-19   19-20   20-21   21-22
isolated ring systems :

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containing 1 : 17 :


Match level :
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Stereo Bonds:

36-9 (Single Hash).


Stereo Chiral Centers:

9      (Parity=Don't Care)

Stereo RSS Sets:

Type=Relative (Default). 1 Nodes= 9
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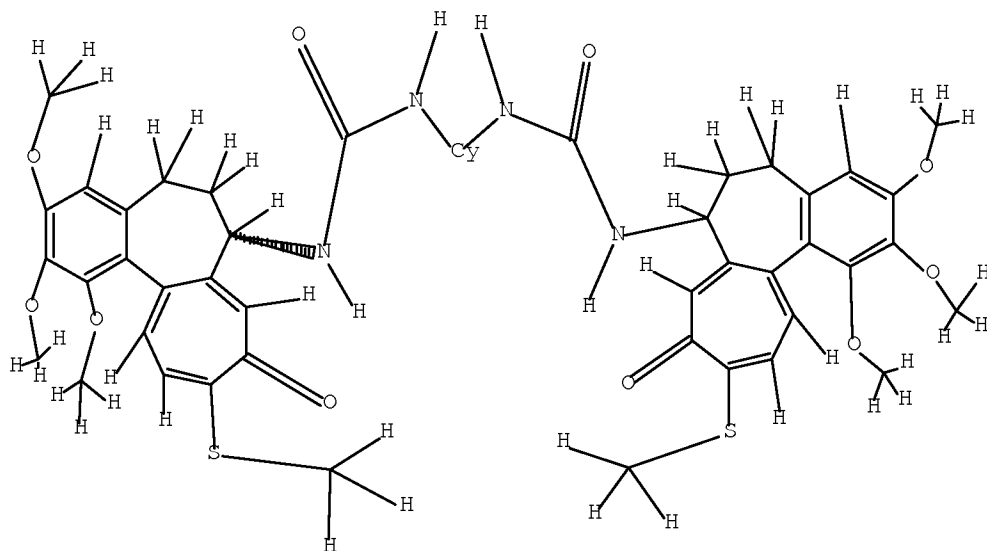
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                                                 ENTRY      SESSION
FULL ESTIMATED COST                               1.35       378.92


DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
                                                 ENTRY      SESSION
CA SUBSCRIBER PRICE                               0.00        -2.34
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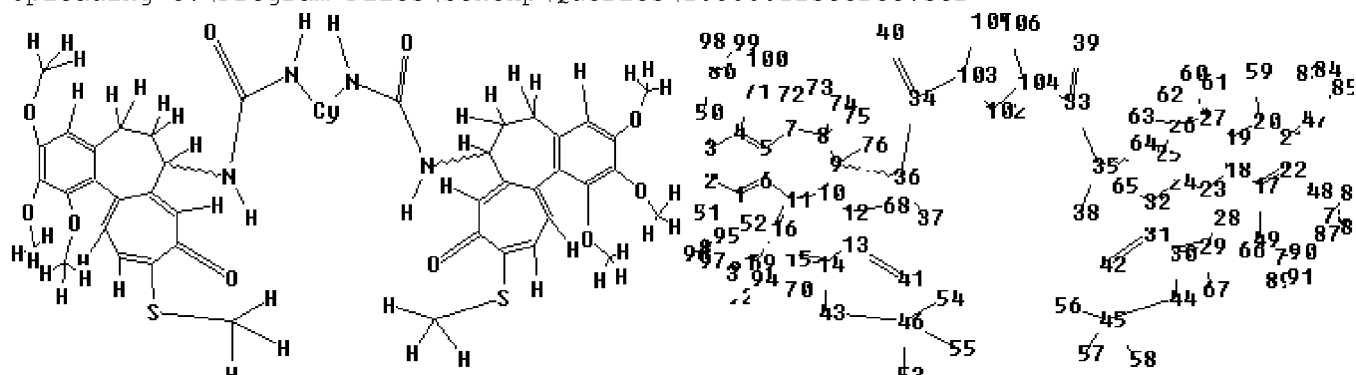TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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chain nodes :
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54   55   56   57   58   59   60   61   62   63   64   65   66   67   68   69   70   71   72   73   74
75   76   77
78   79   80   81   82   83   84   85   86   87   88   89   90   91   92   93   94   95   96   97   98
99   100   102   103
104   105   106
ring nodes :
1    2    3    4    5    6    7    8    9    10   11   12   13   14   15   16   17   18   19   20   21   22   23
24   25   26   27   28   29   30   31   32
chain bonds :
1-52   2-51   3-50   4-71   7-72   7-73   8-74   8-75   9-36   9-76   12-68   13-41   14-43
15-70   16-69   17-49   20-59   21-47   22-48   25-35   25-64   26-62   26-63   27-60   27-61
28-66   29-67   30-44
31-42   32-65   33-39   33-35   33-104   34-40   34-36   34-103   35-38   36-37   43-46   44-
45   45-56
45-57   45-58   46-53   46-54   46-55   47-77   48-78   49-79   50-80   51-82   52-81   77-83
77-84   77-85   78-86
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82-96   82-97
102-103   102-104   103-105   104-106
ring bonds :
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13-14   14-15   15-16   17-18   17-22   18-19   18-23   19-20   19-27   20-21   21-22   23-24
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exact/norm bonds :
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39
33-35   33-104   34-40   34-36   34-103   43-46   44-45   47-77   48-78   49-79   50-80   51-
82   52-81
102-103   102-104
exact bonds :
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78-87   78-88
79-89   79-90   79-91   80-98   80-99   80-100   81-92   81-93   81-94   82-95   82-96   82-97
103-105   104-106
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normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 17-18 17-22 18-19 19-20 20-21 21-22
isolated ring systems :
containing 1 : 17 :


Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom   10:Atom
11:Atom   12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:Atom   18:Atom   19:Atom
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L8   STRUCTURE UPLOADED

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L8 HAS NO ANSWERS
L8   STR
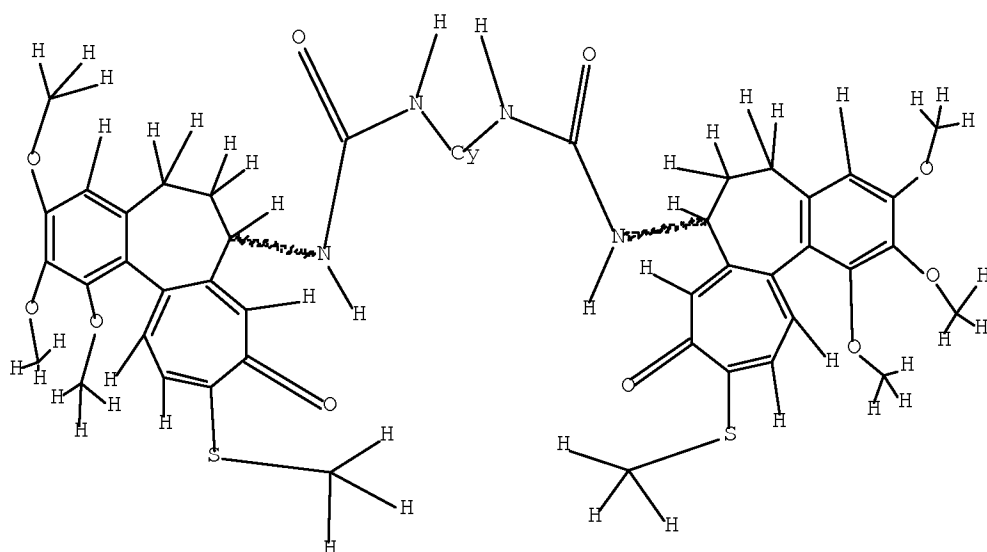
Structure attributes must be viewed using STN Express query preparation.

=> s l8 full
FULL SEARCH INITIATED 18:26:34 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   3 TO ITERATE

100.0% PROCESSED   3 ITERATIONS   2 ANSWERS
SEARCH TIME: 00.00.01

L9   2 SEA SSS FUL L8

=> file caplus
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                       ENTRY   SESSION
FULL ESTIMATED COST   172.55   551.47

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)   SINCE FILE   TOTAL
                                                       ENTRY   SESSION
CA SUBSCRIBER PRICE   0.00   -2.34

=> s l9 full
L10   1 L9

=> d ibib abs hitstr

L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:823659 CAPLUS Full-text
DOCUMENT NUMBER: 143:212050
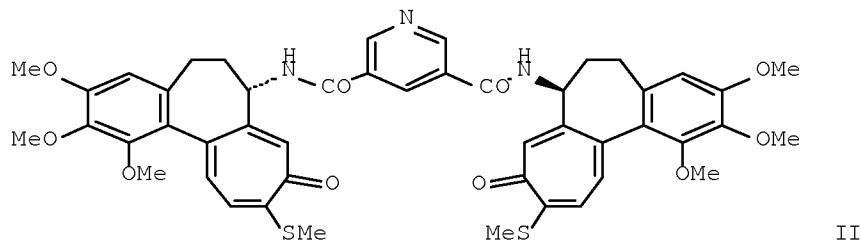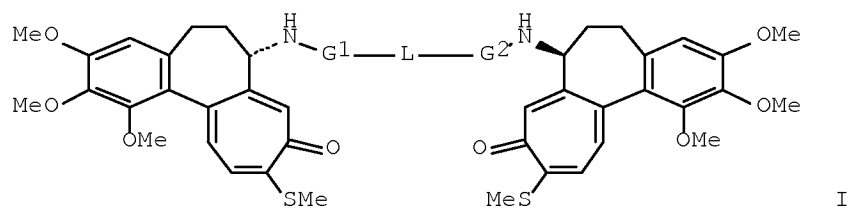TITLE: Preparation of N-deacetylthiocolchicine derivatives
                           for use in antiproliferative, anti-inflammatory,
                           antiarthritic and antiviral pharmaceutical
                           compositions
INVENTOR(S):   Bombardelli, Ezio; Fontana, Gabriele
PATENT ASSIGNEE(S):   Indena S.p.A., Italy

I

II

AB   N-Deacetylthiocolchicine derivs., such as I [G1 = -CO-, -CONH-, -CR2-; G2 = -
     CO-, -NHCO-, -CR2-; L = linking group, such as alkylene, phenylene,
     cyclohexanediyl, pyridinediyl, piperidinediyl, piperazinediyl; R = H, alkyl],
     were prepared for therapeutic use as antitumor, antiproliferative, anti-
     inflammatory, antiarthritic and antiviral agents. Thus, N-
     deacetylthiocolchicine derivative II was prepared via an amidation reaction of
     N-deacetylthiocolchicine with 3,5-pyridinedicarboxylic acid using DMAP and DCC
     in CH2Cl2. The prepared N-deacetylthiocolchicine derivs. were assayed for
     cytotoxic activity against human cancer cell lines, such as MCF7 breast cancer
     cells and A2780 ovarial cancer cells.
IT   862502-68-9P 862502-69-0P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
         (preparation of N-deacetylthiocolchicine derivs. for use in
         antiproliferative, anti-inflammatory, antiarthritic and antiviral
         pharmaceutical compns.)
RN   862502-68-9 CAPLUS
CN   Urea, N,N''-1,4-phenylenebis[N'-[(7S)-5,6,7,9-tetrahydro-1,2,3-trimethoxy-
     10-(methylthio)-9-oxobenzo[a]heptalen-7-yl]- (9CI) (CA INDEX NAME)
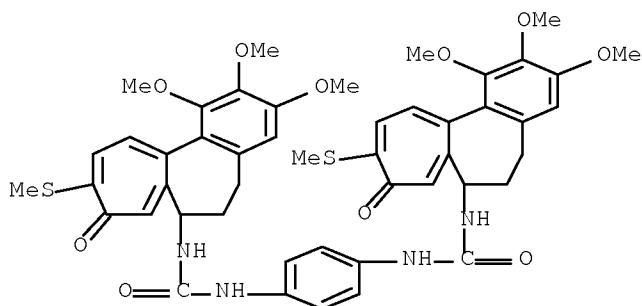
RN   862502-69-0 CAPLUS
CN   Urea, N,N''-1,3-phenylenebis[N'-[(7S)-5,6,7,9-tetrahydro-1,2,3-trimethoxy-
     10-(methylthio)-9-oxobenzo[a]heptalen-7-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

_OMe

————OMe

OMe

```
=> file reg
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                ENTRY       SESSION
FULL ESTIMATED COST                              6.68        558.15

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
                                                ENTRY       SESSION
CA SUBSCRIBER PRICE                             -0.78         -3.12
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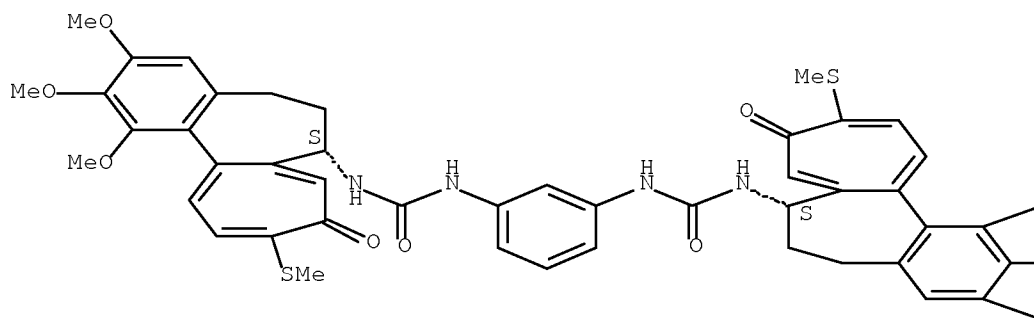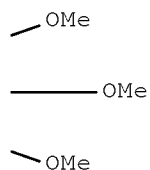
FILE 'REGISTRY' ENTERED AT 18:28:19 ON 17 DEC 2007
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 16 DEC 2007   HIGHEST RN 958294-65-0
DICTIONARY FILE UPDATES: 16 DEC 2007   HIGHEST RN 958294-65-0

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\105880121ast.str

chain nodes :
33   34   35   36   37   38   39   40   41   42   43   44   45   46   47   48   49   50   51   52   53
54   55   56   57   58   59   60   61   62   63   64   65   66   67   68   69   70   71   72   73   74
75   76   77
78   79   80   81   82   83   84   85   86   87   88   89   90   91   92   93   94   95   96   97   98
99   100   102

ring nodes :
1   2   3   4   5   6   7   8   9   10   11   12   13   14   15   16   17   18   19   20   21   22   23
24   25   26   27   28   29   30   31   32

chain bonds :
1-52   2-51   3-50   4-71   7-72   7-73   8-74   8-75   9-36   9-76   12-68   13-41   14-43
15-70   16-69   17-49   20-59   21-47   22-48   25-35   25-64   26-62   26-63   27-60   27-61
28-66   29-67   30-44
31-42   32-65   33-39   33-35   33-102   34-40   34-36   34-102   35-38   36-37   43-46   44-45   45-56
45-57   45-58   46-53   46-54   46-55   47-77   48-78   49-79   50-80   51-82   52-81   77-83
77-84   77-85   78-86
78-87   78-88   79-89   79-90   79-91   80-98   80-99   80-100   81-92   81-93   81-94   82-95
82-96   82-97

ring bonds :
1-2   1-6   2-3   3-4   4-5   5-6   5-7   6-11   7-8   8-9   9-10   10-11   10-12   11-16   12-13
13-14   14-15   15-16   17-18   17-22   18-19   18-23   19-20   19-27   20-21   21-22   23-24
23-28   24-25
24-32   25-26   26-27   28-29   29-30   30-31   31-32

exact/norm bonds :
1-52   2-51   3-50   9-36   13-41   14-43   17-49   21-47   22-48   25-35   30-44   31-42   33-39
33-35   33-102   34-40   34-36   34-102   43-46   44-45   47-77   48-78   49-79   50-80   51-82   52-81

exact bonds :
4-71   5-7   6-11   7-8   7-72   7-73   8-9   8-74   8-75   9-10   9-76   10-11   10-12   11-16
12-13   12-68   13-14   14-15   15-16   15-70   16-69   18-23   19-27   20-59   23-24   23-28
24-25   24-32
25-26   25-64   26-27   26-62   26-63   27-60   27-61   28-29   28-66   29-30   29-67   30-31
31-32   32-65
35-38   36-37   45-56   45-57   45-58   46-53   46-54   46-55   77-83   77-84   77-85   78-86
78-87   78-88
79-89   79-90   79-91   80-98   80-99   80-100   81-92   81-93   81-94   82-95   82-96   82-97

normalized bonds :
1-2   1-6   2-3   3-4   4-5   5-6   17-18   17-22   18-19   19-20   20-21   21-22

isolated ring systems :
containing 1 : 17 :

```
Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom   10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom
20:Atom  21:Atom
22:Atom  23:Atom  24:Atom  25:Atom  26:Atom  27:Atom  28:Atom  29:Atom  30:Atom
31:Atom  32:Atom
33:CLASS  34:CLASS  35:CLASS  36:CLASS  37:CLASS  38:CLASS  39:CLASS  40:CLASS
41:CLASS  42:CLASS
43:CLASS  44:CLASS  45:CLASS  46:CLASS  47:CLASS  48:CLASS  49:CLASS  50:CLASS
51:CLASS  52:CLASS
53:CLASS  54:CLASS  55:CLASS  56:CLASS  57:CLASS  58:CLASS  59:CLASS  60:CLASS
61:CLASS  62:CLASS
63:CLASS  64:CLASS  65:CLASS  66:CLASS  67:CLASS  68:CLASS  69:CLASS  70:CLASS
71:CLASS  72:CLASS
73:CLASS  74:CLASS  75:CLASS  76:CLASS  77:CLASS  78:CLASS  79:CLASS  80:CLASS
81:CLASS  82:CLASS
83:CLASS  84:CLASS  85:CLASS  86:CLASS  87:CLASS  88:CLASS  89:CLASS  90:CLASS
91:CLASS  92:CLASS
93:CLASS  94:CLASS  95:CLASS  96:CLASS  97:CLASS  98:CLASS  99:CLASS  100:CLASS
102:Atom


L11       STRUCTURE UPLOADED

=> d l11
L11 HAS NO ANSWERS
L11               STR
```
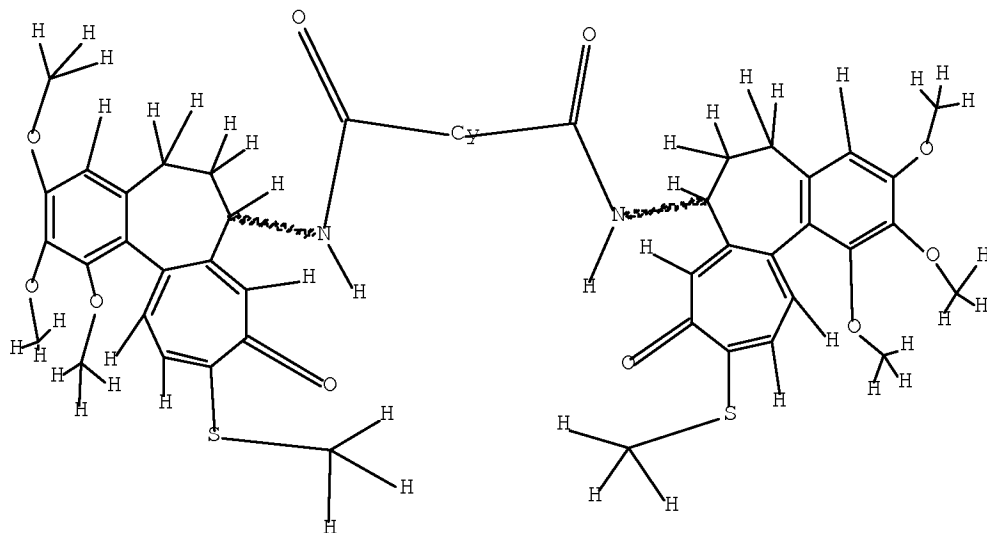


```
Structure attributes must be viewed using STN Express query preparation.


=> s l11 full
FULL SEARCH INITIATED 18:29:29 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -       51 TO ITERATE
```

```
100.0% PROCESSED       51 ITERATIONS                         4 ANSWERS
SEARCH TIME: 00.00.01


L12            4 SEA SSS FUL L11

=> file capluis
'CAPLUIS' IS NOT A VALID FILE NAME
SESSION CONTINUES IN FILE 'REGISTRY'
Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files
that are available.  If you have requested multiple files, you can
specify a corrected file name or you can enter "IGNORE" to continue
accessing the remaining file names entered.

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE       TOTAL
                                                ENTRY         SESSION
FULL ESTIMATED COST                            172.55         730.70


DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE       TOTAL
                                                ENTRY         SESSION
CA SUBSCRIBER PRICE                              0.00          -3.12

FILE 'CAPLUS' ENTERED AT 18:29:37 ON 17 DEC 2007
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FILE LAST UPDATED: 16 Dec 2007  (20071216/ED)

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=> s l12 full
L13            2 L12

=> d his

     (FILE 'HOME' ENTERED AT 18:00:07 ON 17 DEC 2007)

     FILE 'REGISTRY' ENTERED AT 18:00:12 ON 17 DEC 2007
L1              STRUCTURE UPLOADED
L2              1 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 18:01:09 ON 17 DEC 2007
L3              1 S L2 FULL
```

```
        FILE 'REGISTRY' ENTERED AT 18:13:39 ON 17 DEC 2007
L4              STRUCTURE UPLOADED
L5              4 S L4 FULL


        FILE 'CAPLUS' ENTERED AT 18:14:23 ON 17 DEC 2007
L6              2 S L5 FULL


        FILE 'REGISTRY' ENTERED AT 18:22:53 ON 17 DEC 2007


        FILE 'REGISTRY' ENTERED AT 18:23:43 ON 17 DEC 2007
L7              STRUCTURE UPLOADED


        FILE 'REGISTRY' ENTERED AT 18:25:27 ON 17 DEC 2007
L8              STRUCTURE UPLOADED
L9              2 S L8 FULL


        FILE 'CAPLUS' ENTERED AT 18:26:47 ON 17 DEC 2007
L10             1 S L9 FULL


        FILE 'REGISTRY' ENTERED AT 18:28:19 ON 17 DEC 2007
L11             STRUCTURE UPLOADED
L12             4 S L11 FULL


        FILE 'CAPLUS' ENTERED AT 18:29:37 ON 17 DEC 2007
L13             2 S L12 FULL

=> log y
COST IN U.S. DOLLARS                      SINCE FILE      TOTAL
                                            ENTRY        SESSION
FULL ESTIMATED COST                          0.47        731.17

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)  SINCE FILE      TOTAL
                                            ENTRY        SESSION
CA SUBSCRIBER PRICE                          0.00         -3.12

STN INTERNATIONAL LOGOFF AT 18:29:47 ON 17 DEC 2007
```